

BY Pho Student Noor Taba Ismaee supervisor

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Combinatorial Preparation and Characterization **Methods for High Through-put Study of Advanced Functional** Materials



Aim of the

sputtering.



We prepared thin films of mixed Titanium Oxide and Molybdenum Trioxide (TiO2-MoO3) mixed layers on glass by reactive DC magnetron sputtering and determined the optimal composition for electrochromic purposes. We mapped the composition and optical parameters by using **Spectroscopic Ellipsometry (SE).**

Research Work





a) b) Figure (1) a) arrangements of the two targets in closer position (35 cm from each other); b) the chamber for DC magnetron sputtering device after air vacuumed. Blue light is from the Ar-O₂ plasma gas mixture.



Figure (2) Spectroscopic Ellipsometry device, Woollam M-2000DI.

Electrochromic measurements have been performed to optimize the composition of (TiO2-MoO3) mixed layers. The mixed oxide film was deposited onto the Indium-Tin-Oxide surface (ITO) covered glass.

Optical parameters and composition have been determined and mapped by using Spectroscopic Ellipsometry (SE). Scanning Electron Microscopy (SEM) with Energy-Dispersive X-ray Spectroscopy (EDS) has been used to check the SE results see Fig. 8.

The main standard of the EC device performance is Coloration Efficiency η (CE, the change of light transmission for the same electric charge) of mixed metal oxides (TiO2-MoO3) has been determined in a transmission electrochemical cell, see Fig. 5



Figure (3) TiO₂-MoO₃, ITO- covered glass and Si-probes on a glass substrate, before-electrochromic-experiments, the Ti-rich in the left side and the Mo-rich in the right side .



Figure (4) TiO₂-MoO₃ after-electrochromic-experiments. Thermal shock can be seen in the Ti-rich side



Figure (5) TiO2-MoO3 during-electrochromicexperiments by SE, to determined CE in a transmission electrochemical cell.



Figure (6) SEM micrograph from the TiO₂-MoO₃ surface Ti-rich-side, Polycrystalline structure can be seen caused by thermal shock.

AX.	HV	curr	det	mode	mag	只	WD	HFW	use case	PW	tilt	1 μm
X	10.00 kV	1.6 nA	ETD	SE	20 000	х	7.0 mm	6.35 μm	OptiTilt	4.13 nm	0.0 °	EK MFA

Figure (7) SEM micrograph from the TiO₂-MoO₃ surface Mo-rich-side, it is remained amorphous (or nanocrystalline).

Ti-Mo ratio [%]



Figure (8) Ti/Mo ratio measured on the Si-probes by SEM-EDS. The accuracy of the Ti/Mo ratio is 2 %, while the precision of the position is 1 mm.



Figure (9) Coloration Efficiency of TiO₂-MoO₃. vs. Mo % for wavelengths from (400-800) nm by home-made software version 1.0 coded in Python version 3.11 language. Two peaks can be explained by the microstructure difference on the two sides of the CE curves. Individual color-coded curves represent different wavelengths: 1 - 400 nm, 2 - 500 nm, 3 - 600 nm, 4 - 700 nm, 5 - 800 nm).

Conclusions

By using this combinatorial process, all the compositions (from 0 to 100%) were achieved. The second showed better EC properties than the pure oxides.

The Two peaks can be explained by the microstructure difference on the two sides of the CE curves, Ti-rich side was at significantly higher temperature during the deposition process, so the Ti-rich oxide is polycrystalline compared to the Mo-rich side where the oxide remains amorphous or nanocrystalline. The maximum value of the CE is 22.2 cm²/C at the wavelength 600 nm at ~ 60% - 40 % Ti-Mo ratio on the Ti-rich polycrystalline material, while CE is $19.8 \text{ cm}^2/\text{C}$ at the wavelength 600 nm at ~ 20% - 80 % Ti-Mo ratio on the Mo-rich amorphous (or nanocrystalline) material.

Planned steps forward:-

1. Further investigation of stoichiometric and substoichiometric oxides for gas sensorics purposes see Fig. 10.



Figure (10) Photographs (from different view-angle) of WoO_3/MoO_3 (lower) or WoO_{3-x}/MoO_{3-x} (upper) combinatorial sets on heat-able sensor chips. Inserted photograph shows Pt contacted sample.

1- I submitted an article, and it is now "under review" to the Acta Polytechnica Hungarica Journal on 14 of December 2023. Authors: Noor Taha Ismaeel, Zoltan Labadi and Miklos Fried. Title: Investigation of Combinatorial TiO_2 -MoO₃ Mixed Layers to Optimize the Electrochromic Properties. Number: 6540. You can access it via the Acta1034 EasyChair Web page:

https://easychair.org/conferences/?conf=acta1034

2- I participate and take a certificate from the Budapest School on Modern X-ray Science 2023, 3-6 of October in Research Centre for Natural Sciences (ttk), Budapest. see the images below:

Budapest School on Modern X-ray Science

3-6 October 2023, Budapest, Hungary



Certificate

This document is to certify that NOOR Taha Ismaeel took part in the school of "Budapest School on Modern X-ray Science 2023" held in Budapest at Research Centre for Natural Sciences in 3-6 October 2023.

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György Vankó

Wigner Research Centre for Physics

Budapest, 6 October 2023



3- I presented my research in the XXXIX. Kandó Konferencia 2023, 9-10 of November in ÓbudaI Egyetem 1084 Budapest, Tavaszmező u. 17. see the image below:



4- I attend the 3rd edition of Surface Science Discussions - a free online seminar featuring lectures from well-renowned scientists in the field that takes place on 09-10.01.2024.



Tailoring electrocatalyst performance through the second s

Su-Hyun Yoo Chemical Data-Driven Research Center, Korea Research Institute of Chemical Technology, Korea syoo@krict.re.kr

2024-01-09 | Surface Science Discussion 2024

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Publikációk listája a PhD képzés kezdetétől /

List of publications from the beginning of the training program for NOOR TAHA ISMA

No	Cím / Title	Folyóirat vagy konferencia neve / Name of journal or conference	IF, Q	Összes kredit / Total credit	%
1-	https://ellipsometry.hu/Anyagtudomany- Symp-Matrahaza-2022-10-5-7-ISBN-978- 963-449-320-4-2023.pdf ISBN: 9789634493204	Symposium on Materials Science, Mátraháza, Hungary, October 5-7, 2022		24	100
2-	https://konf2022.kvk.uni-obuda.hu/program ISBN 978-963-449-299-3	XXXVIII. Kandó Conference 2022 November 3-4, 2022		24	100
3-	https://www.mdpi.com/1996- 1944/16/12/4204	Materials Journal 6 June 2023 MDPI	I F 3.748 Q2	36	100
4-	https://doi.org/10.32802/asmscj.2022.1263	ASM Science Journal 09-08- 2022	Scopus		100
5-	https://doi.org/10.32802/asmscj.2022.1215	ASM Science Journal 30-06- 2022	Scopus		100
6-	https://www.iasj.net/iasj/download/bd56f1e 825a3bfa5	Iraqi Journal Of Laser 1-12-2022			100



